Index

Original Investigations and Short Communications

Alagona, G., Scrocco, E., Tomasi, J.: On a Possible Catalytic Effect of Water on Some Nucleophilic Substitution Reactions in "Inert" Solvents . . . 133

Bellagamba, V., Ercoli, R., Gamba, A., Morosi, G.: Calculation of hfs Coupling Constants by the Roothaan "Plus" Configuration Interaction Method within the INDO Approximation . . 329

Berthod, H., Pullman, A.: Quantum-Mechanical Exploration of the Properties of the Sugar Rings. I. Electrostatic Molecular Potential, Hydration and Cation Binding Scheme of C_3-Endo-*gg*-Ribose . . . 59

Berthod, H., s. Pullman, A., et al. . . . 175

Blustin, P. H.: A Floating Gaussian Orbital Calculation on Argon Hydrochloride (Ar·HCl) . . 249

Caillet, J., Claverie, P., Pullman, B.: Effect of the Crystalline Environment upon the Rotational Conformation about the N—C and C—C' Bonds (Φ and Ψ) in Amides and Peptides . . . 17

Chung, K.-M., s. Hartmann, H. . . . 147

Claverie, P., s. Caillet, J., et al. . . . 17

Cooper, I. L., Pounder, C. N. M.: The Analysis of Electron Pair Distribution Functions in Molecules 51

Csizmadia, I. G., s. Hopkinson, A. C., et al. . . . 97

Diercksen, G. H. F., s. Hennig, P., et al. . . . 233

Ercoli, R., s. Bellagamba, V., et al. . . . 329

Fernández-Alonso, J. I., s. Moscardó, F. . . . 305

Gamba, A., s. Bellagamba, V., et al. . . . 329

Goldblum, A., Pullman, B.: Study of Anion Binding to Protonated Nucleic Acid Bases Using Electrostatic Molecular Potentials . . . 345

Golding, R. M., s. Macdonald, J. R. . . . 1

Gutman, I.: Bounds for Reactivity Indices . . . 217

Hartmann, H., Chung, K.-M.: On the Application of a Classical Perturbation Theory to the Theory of Coupled Fields . . . 147

Hennig, P., Kraemer, W. P., Diercksen, G. H. F., Strey, G.: SCF-CI Studies on the Electronic Ground State of Water: Potential Energy Hypersurface and Spectroscopic Constants . . . 233

Hopkinson, A. C., Lien, M. H., Csizmadia, I. G., Yates, K.: Quantum Chemical Studies on Electrophilic Addition. III. Reaction of Hydroxonium Ion with Ethylene. Acid Catalysed Ring Opening of Epoxides . . . 97

Howell, J. M., s. Olsen, J. F. . . . 39

Jankowski, K., Muszyńska, J., Rutkowski, A.: An Investigation of the Reliability of the Galerkin-Petrov Method. II. Ground-State of the Beryllium Atom . . . 275

Kitaura, K., s. Yamabe, S., et al. . . . 111

Klessinger, M., Schmidt, W.: VB Calculations with Orthogonal Basis Functions. I. Minimal Basis *ab initio* Calculations . . . 193

Kraemer, W. P., s. Hennig, P., et al. . . . 233

Krogh-Jespersen, K., Ratner, M. A.: Application of a Screened INDO Model (INDO/S) to Spectroscopic Properties of TCNQ and Its Anions . . . 283

Lien, M. H., s. Hopkinson, A. C., et al. . . . 97

Macdonald, J. R., Golding, R. M.: An Examination of UHF Methods for Atoms in the First Three Rows . . . 1

Meinköhn, D.: On the Investigation of Pseudoscalar Molecular Properties and Polynomial Approximations According to Ruch and Schönhofer . . . 67

Meyer, A. Y., Pasternak, R.: Molecular-Orbital Realizations of the Bent-Bond Model: Spiranic Derivatives of Cyclobutanone . . . 27

Mó, O., Yáñez, M.: Influence of Polarization Functions on Molecular Electrostatic Potentials . . 263

Morosi, G., s. Bellagamba, V., et al. . . . 329

Moscardó, F., Fernández-Alonso, J. I.: Role of Coupling Operators on Open Shell RHF Equations . . . 305

Muszyńska, J., s. Jankowski, K., et al. . . . 275
Nishimoto, K., s. Yamabe, S., et al. . . . 111
Olsen, J. F., Howell, J. M.: *Ab initio* Studies on Several Species of the Formula X_3YO and X_3YOH. Geometries and Electronic Structures . . . 39
Ovchinnikov, A. A.: Multiplicity of the Ground State of Large Alternant Organic Molecules with Conjugated Bonds . . . 297
Pasternak, R., s. Meyer, A. Y. . . . 27
Poulain, E., s. Tapia, O., et al. . . . 171
Pounder, C. N. M., s. Cooper, I. L. . . . 51
Pullman, A., s. Berthod, H. . . . 59
Pullman, A., Pullman, B., Berthod, H.: An SCF *ab initio* Investigation of the "Through-Water" Interaction of the Phosphate Anion with the Na^+ Cation . . . 175
Pullman, B., s. Caillet, J., et al. . . . 17
Pullman, B., s. Pullman, A., et al. . . . 175
Pullman, B., s. Goldblum, A. . . . 345
Ratner, M. A., s. Krogh-Jespersen, K. . . . 283
Reschke, R., Trautwein, A.: Numerical Integration of Overlap and Ligand Contributions to the Electric Field Gradient . . . 85
Rutkowski, A., s. Jankowski, K., et al. . . . 275
Sadlej, A. J.: Molecular Electric Polarizabilities. II. Static Polarizabilities of Diatomic Molecules Using 2-ζ Quality EFV GTO Basis Set . . . 205
Schmidt, W., s. Klessinger, M. . . . 193
Scrocco, E., s. Alagona, G., et al. . . . 133
Spanget-Larsen, J.: INDO Calculations with Inclusion of an Effective Solvent Field. Application to Benzosemiquinones . . . 315
Strey, G., s. Hennig, P., et al. . . . 233
Summers, N. L., Tyrell, J.: *Ab initio* Studies of the Protonation of CO, N_2, and NO^+: Calculation of the Minimum Energy Reaction Paths . . . 223
Sussman, F., s. Tapia, O., et al. . . . 171
Tapia, O.: Some Remarks on the SCRF Theory of Solvent Effects and the Calculation of Proton Potentials 157
Tapia, O., Poulain, E., Sussman, F.: Environmental Effects on Second Order Perturbation Energy 171
Tomasi, J., s. Alagona, G., et al. . . . 133
Trautwein, A., s. Reschke, R. . . . 85
Tyrrell, J., s. Summers, N. L. . . . 223
Yamabe, S., Kitaura, K., Nishimoto, K.: A MO-Theoretical Study of the Hydrogen Bond in $(HCOOH)_2$, $(HCONH_2)_2$, and $(B(OH)_3)_2$ . . . 111
Yáñez, M., s. Mó, O. . . . 263
Yates, K., s. Hopkinson, A. C., et al. . . . 97

Book Reviews

Csizmadia, I. G. (Ed.): Applications of MO Theory in Organic Chemistry (Ref. Preuss, H.) . . . 349
Goodisman, J.: Contemporary Quantum Chemistry (Ref. Jug, K.) . . . 259
Parr, R. G., s. Pullman, B. . . . 81
Pullman, B., Parr, R. G.: The New World of Quantum Chemistry (Ref. Fernández-Alonso, J. I.) . . . 81
Silver, B. L., (Ed.): Irreducible Tensor Methods. An Introduction for Chemists (Ref. Bingel, W. A.) . 260
Wagnière, G. H.: Introduction to Elementary Molecular Orbital Theory and to Semiempirical Methods (Ref. Schmidtke, H.-H.) . . . 83

Indexed in Current Contents

Subject Index

Argon hydrochloride (Ar·HCl) 249

Benzosemiquinones, spin densities and geometries of ~ 315
Beryllium 275
Bivariational procedures 275

C_3,-endo ribose 59
Carbonyl stretching frequency 27
Catalytic effects 133
Chirality functions 67
Classical perturbation theory 147
Coupled fields 147
Crystalline environment 17

Dispersion forces 171

Electric field gradient, total, calculation of ~ 85
Electric field variant Gaussian orbitals 205
Electron correlation 275
Electron pair distribution 51
Electronic structure of X_3YO type compounds 39
Energy decomposition 111
Epoxides, acid catalysed ring opening of ~ 97

Formamide dimer 111
Formic acid dimer 111
Free valence 217

Graph theory 217

Heterolytic cleavage 133
hfs constants 329
Homochirality 67
Hybrids, linear combination of ~ 27
Hydrogen bond 111
Hydrogen bonded complexes 133
Hydroxonium ion, reaction of ~ with ethylene 97

INDO method with a contribution from the solvent 315

Localization energy 217

Method of moments, reliability of ~ 275
Molecular dipole moments 205
Molecular electrostatic potentials 263
Molecular polarizabilities 205

Nucleic acid bases, protonated, anion binding to ~ 345

Open-shell theory 305
Organic molecules, large alternant ~ 297
Organic radicals 329
Orthoboric acid dimer 111

Phosphate anion, interaction with Na^+ cation 175
Polarizability 217
Polarization functions 263
Proton potentials 157
Φ and Ψ torsion angles in amides and peptides 17

Reaction paths, minimum energy ~, for formation of HCO^+, COH^+, $HCOH^{2+}$ by protonation 223
Resonance Raman spectroscopy 283
RHF + CI method 329
RHF equations 305
Rotational conformation in amides and peptides 17

Saturated organic compounds, MO treatment of ~ 27
SCF perturbation theory 205
Screened INDO model 283
Self-consistent reaction field 157
Small rings 27
Solvent effect 157, 171
Sugar rings, quantum mechanical exploration of ~ 59

TCNQ and its anions 283
Theory of invariants 67
Through water interaction 175

UHF methods, reliability and usefulness of ~ 1

Van der Waals molecules 249
VB method 193

Water molecule, electronic ground state of ~ 233

Instructions to Authors

Manuscripts should be *submitted in duplicate*, typed in double-line spacing on one side of the paper only. Form and contents should be carefully checked to exclude the need for corrections in proof. The author should already mark in the manuscript where figures and tables are to be inserted, as he will receive only *one set of proofs* to correct typographical errors. Authors will be charged for corrections in proof involving changes, additions, or deletions to the original manuscript.

The papers should be preceded by an *English summary* of not more than 100 words. Papers not written in English should have an English translation of the title.

Immediately following the summary, a list of *Key words* (not exceeding five items normally) should be supplied for subject indexing.

Literature references should be numbered and listed at the end of the paper. They should be cited as follows: *journal papers* — names and initials of all authors, journal with abbreviations according to the I.U.P.A.C. list (Chemical Abstracts, Vol. 55, 1961), volume and page number, year in parentheses; *books* — names of authors, full title, edition, place, publisher and year. References should be cited in the text by number.

Figures, graphs, tables and structural formulae should be separated from the text and be numbered. Original drawings and graphs should be made in Indian ink with lines of uniform thickness. Authors should keep in mind that drawings will be reduced to a size not exceeding 12 × 19 cm. In general it should be assumed that the same degree of reduction will apply to all figures in the same paper. Inscriptions should allow for any reduction in scale — a capital letter should be about 1.8 mm in height in the final version. Computer print-outs should be black and evenly printed to allow direct reproduction.

Captions, which should be brief, should be typed separately and attached to the manuscript.

Formulae should be typewritten, special attention being given to the placing of indices and exponents to that they are recognizable as such even though there is no difference in size. Formulae should preferably be written in a "linear" form e. g. $\exp(-\varepsilon/kT)$ instead of $e^{\frac{\varepsilon}{kT}}$). It will help the printer if in doubtful cases the position of indices and exponents is marked thus: $b_{\uparrow}$, $a^{\downarrow}$.

Underlining for special alphabets and typefaces should be done according to the following code:

violet:	numerals to be distinguished from letters (1, *l*; zero, *O*)		
single underlining:	small letter		
double underlining:	capital letter	red:	Greek
brown:	boldface	blue:	Gothic
yellow:	upright	green:	Script

The following are frequently confused:

$\cup, \mathrm{u}, \bigcup, U$; $\circ, o, O, 0$; $\times, x, X, \varkappa$; $\vee, v, \nu$; $\theta, \Theta, \phi, \varphi, \Phi, \varnothing, \emptyset$; ψ, Ψ; $\varepsilon, \in$;

a', a^1; the symbol *a* and the indefinite article a. Please take care to distinguish them in some way.

Special alphabets or typefaces

Script	$\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}, \mathcal{E}, \mathcal{F}, \mathcal{G}, \mathcal{H}, \mathcal{I}, \mathcal{J}, \mathcal{K}, \mathcal{L}, \mathcal{M}, \mathcal{N}, \mathcal{O}, \mathcal{P}, \mathcal{Q}, \mathcal{R}, \mathcal{S}, \mathcal{T}, \mathcal{U}, \mathcal{V}, \mathcal{W}, \mathcal{X}, \mathcal{Y}, \mathcal{Z}$
	$a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p, q, r, s, t, u, v, w, x, y, z$
Sanserif	A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z
	a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p, q, r, s, t, u, v, w, x, y, z
Boldface, italic	$\boldsymbol{A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z}$
	$\boldsymbol{a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p, q, r, s, t, u, v, w, x, y, z}$
Special Roman	$\mathbb{A}, \mathbb{B}, \mathbb{C}, \mathbb{D}, \mathbb{E}, \mathbb{F}, \mathbb{G}, \mathbb{H}, \mathbb{I}, \mathbb{J}, \mathbb{K}, \mathbb{L}, \mathbb{M}, \mathbb{N}, \mathbb{O}, \mathbb{P}, \mathbb{Q}, \mathbb{R}, \mathbb{S}, \mathbb{T}, \mathbb{U}, \mathbb{V}, \mathbb{W}, \mathbb{X}, \mathbb{Y}, \mathbb{Z}, \mathbb{1}$
Greek	$\Gamma, \Delta, \Theta, \Lambda, \Xi, \Pi, \Sigma, \Phi, \Psi, \Omega$
	$\alpha, \beta, \gamma, \delta, \varepsilon, \zeta, \eta, \theta, \vartheta, \iota, \kappa, \lambda, \mu, \nu, \xi, o, \pi, \rho, \sigma, \tau, \upsilon, \varphi, \phi, \chi, \psi, \omega$

Notations

preferred form	instead of	preferred form	instead of
$A^*, b^{\sim}, \gamma', \mathbf{v}$	$\bar{A}, \hat{b}, \check{\gamma}, \vec{v}$	$f: A \to B$	$A \xrightarrow{f} B$
lim sup, lim inf	$\overline{\lim}, \underline{\lim}$		
inj lim, proj lim	$\varinjlim, \varprojlim$		
$\exp(-(x^2+y^2)/a^2)$	$e^{\frac{-x^2+y^2}{a^2}}$	$\dfrac{\cos(1/x)}{(a+b/x)^{1/2}}$	$\cos\dfrac{1}{x}$ $\overline{\sqrt{a+\dfrac{b}{x}}}$
f^{-1}	$\overset{-1}{f}$		

THEORETICA CHIMICA ACTA

Manuscripts may be submitted to the Editor-in-Chief, to any of the Co-editors listed below, or to the Editorial Office

Australia
Prof. Dr. Ronald D. Brown,
Department of Chemistry, Monash University, P. O. Box 92, Clayton, Victoria, 3168

Austria
Prof. Dr. A. Neckel,
Institut für Technische Elektrochemie,
Technische Hochschule Wien, Getreidemarkt 9, A-1060 Wien

Canada
Prof. Dr. Camille Sandorfy,
Université de Montréal, Case Postale 6128, Montréal

Czechoslovakia
Prof. Dr. Rudolf Zahradník,
J.-Heyrovský-Institute of Physical Chemistry and Electrochemistry,
Czechoslovak Academy of Sciences, Máchova 7, 12138 Prague 2

Denmark
Prof. Dr. Carl J. Ballhausen,
Chemical Laboratory IV, H. C. Ørstedinstitutet, Universitetsparken 5,
København Ø

France
Prof. Dr. Bernard Pullman,
Institut de Biologie Physico-Chimique, Université de Paris, 13 rue Pierre et Marie Curie, F-75005 Paris

Germany
Prof. Dr. R. Gleiter,
Institut für Organische Chemie, Technische Hochschule, Darmstadt,
Petersenstr. 22, D-6100 Darmstadt

Prof. Dr. Jaroslav Koutecký,
Institut für physikalische Chemie und Quantenchemie, Freie Universität Berlin,
Thielallee 63–67, D-1000 Berlin 33

Great Britain
Prof. Dr. G. G. Hall,
Department of Mathematics, University of Nottingham, University Park,
Nottingham

Israel
Dr. E. A. Halevi,
Technion - Israel Institute of Technology,
Department of Chemistry, Haifa 32000

Prof. Dr. Joshua Jortner,
Institute of Chemistry, Tel-Aviv University, Ramat-Aviv, Tel-Aviv

Italy
Prof. Dr. Massimo Simonetta,
Istituto di Chimica Fisica dell'Università di Milano, Via Golgi 19, Milano

Japan
Prof. Dr. Masao Kotani,
36-4 Sanno 3 chome, Ota-ku, Tokyo 143

Prof. Dr. Kenichi Fukui,
Department of Hydrocarbon Chemistry, Faculty of Engineering, Kyoto University, Kyoto

Sweden
Prof. Dr. Bengt Rånby,
The Royal Institute of Technology, Department of Polymer Technology,
Teknikringen 44, S-100 44 Stockholm 70

Switzerland
Prof. Dr. Edgar Heilbronner,
Physikalisch-Chemisches Institut der Universität Basel, Klingelbergstraße 80,
CH-4000 Basel

USA
Prof. Dr. Ralph G. Pearson,
Chemistry Department, University of California, Santa Barbara, CA 93106

Prof. Dr. Klaus Ruedenberg,
Department of Chemistry, Iowa State University of Science and Technology,
Ames, IA 50010

Prof. Dr. Oktay Sinanoğlu,
Department of Chemistry, Yale University, 225 Prospect Street, New Haven,
CT 06520

USSR
Prof. Dr. E. E. Nikitin,
Institute of Chemical Physics, Academy of Sciences of the USSR,
Vorobyevskoye chaussée 2-b, Moskwa V-334

THEORETICA CHIMICA ACTA

Volume 47 Number 4

Original Investigations

O. Mó, M. Yáñez: Influence of Polarization Functions on Molecular Electrostatic Potentials 263

K. Jankowski, J. Muszyńska, A. Rutkowski: An Investigation of the Reliability of the Galerkin-Petrov Method. II. Ground-State of the Beryllium Atom 275

K. Krogh-Jespersen, M. A. Ratner: Application of a Screened INDO Model (INDO/S) to Spectroscopic Properties of TCNQ and Its Anions 283

A. A. Ovchinnikov: Multiplicity of the Ground State of Large Alternant Organic Molecules with Conjugated Bonds 297

F. Moscardó, J. I. Fernández-Alonso: Role of Coupling Operators on Open Shell RHF Equations 305

J. Spanget-Larsen: INDO Calculations with Inclusion of an Effective Solvent Field. Application to Benzosemiquinones 315

V. Bellagamba, R. Ercoli, A. Gamba, G. Morosi: Calculation of hfs Coupling Constants by the Roothaan "Plus" Configuration Interaction Method within the INDO Approximation 329

Short Communication

A. Goldblum, B. Pullman: Study of Anion Binding to Protonated Nucleic Acid Bases Using Electrostatic Molecular Potentials 345

Book Review

I. G. Csizmadia (Ed.): Applications of MO Theory in Organic Chemistry (Ref. H. Preuss) 349

Indexed in Current Contents